TOPIC 02 – ATOMIC STRUCTURE
2.2: THE MASS SPECTROMETER

IB Chemistry

T02D02

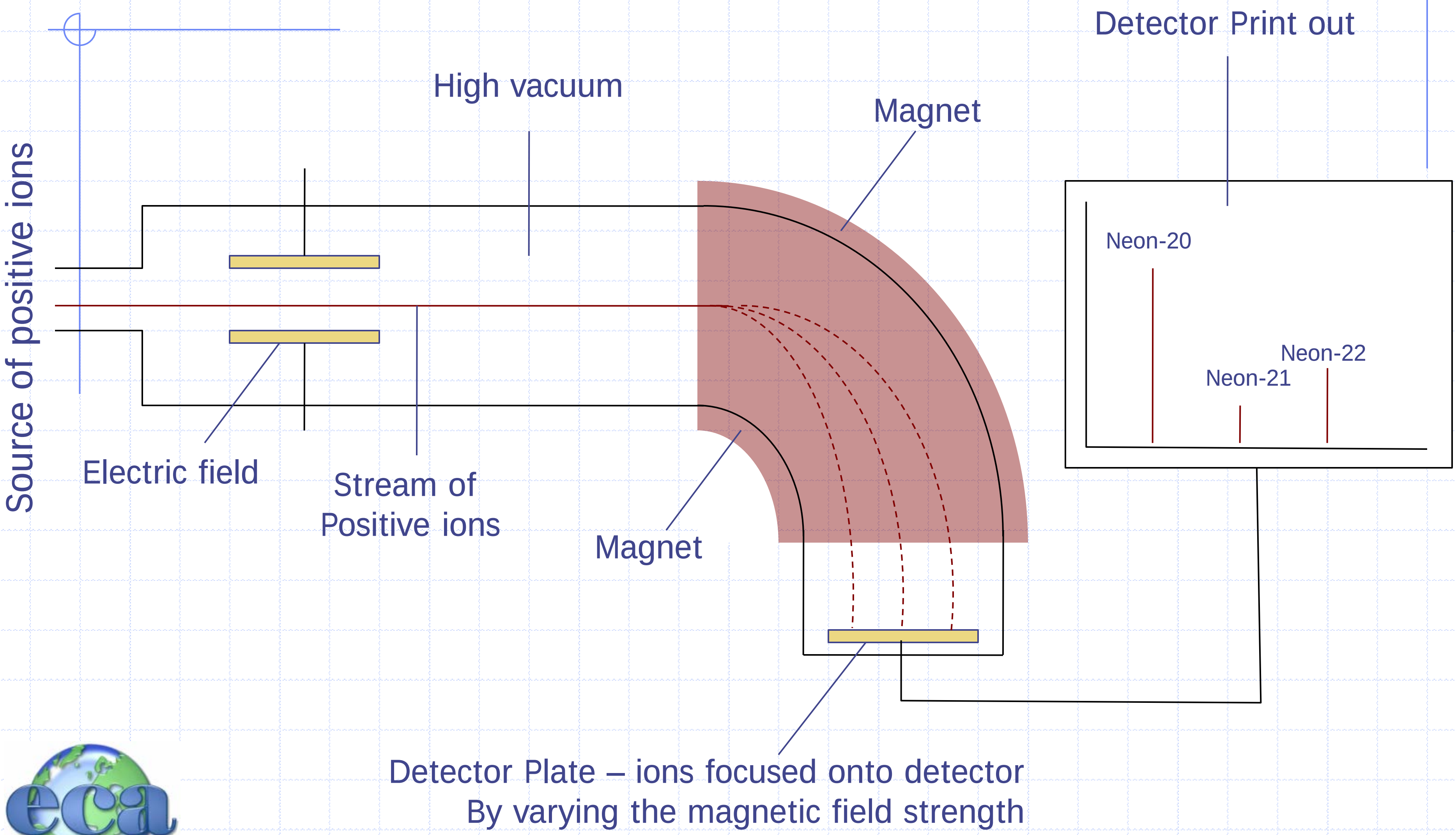
2.1 The Mass Spectrometer - 1 hour

- 2.2.1 Describe and explain the operation of a mass spectrometer. (3)
- 2.2.2 Describe how the mass spectrometer may be used to determine relative atomic mass using the 12C scale. (2)
- 2.2.3 Calculate non-integer relative atomic masses and abundance of isotopes from given data. (2)
- 1.2.4 – Distinguish between the terms empirical formula and molecular formula
- 1.2.5 – Determine the empirical formula from the percentage composition ~~or from other experimental data~~

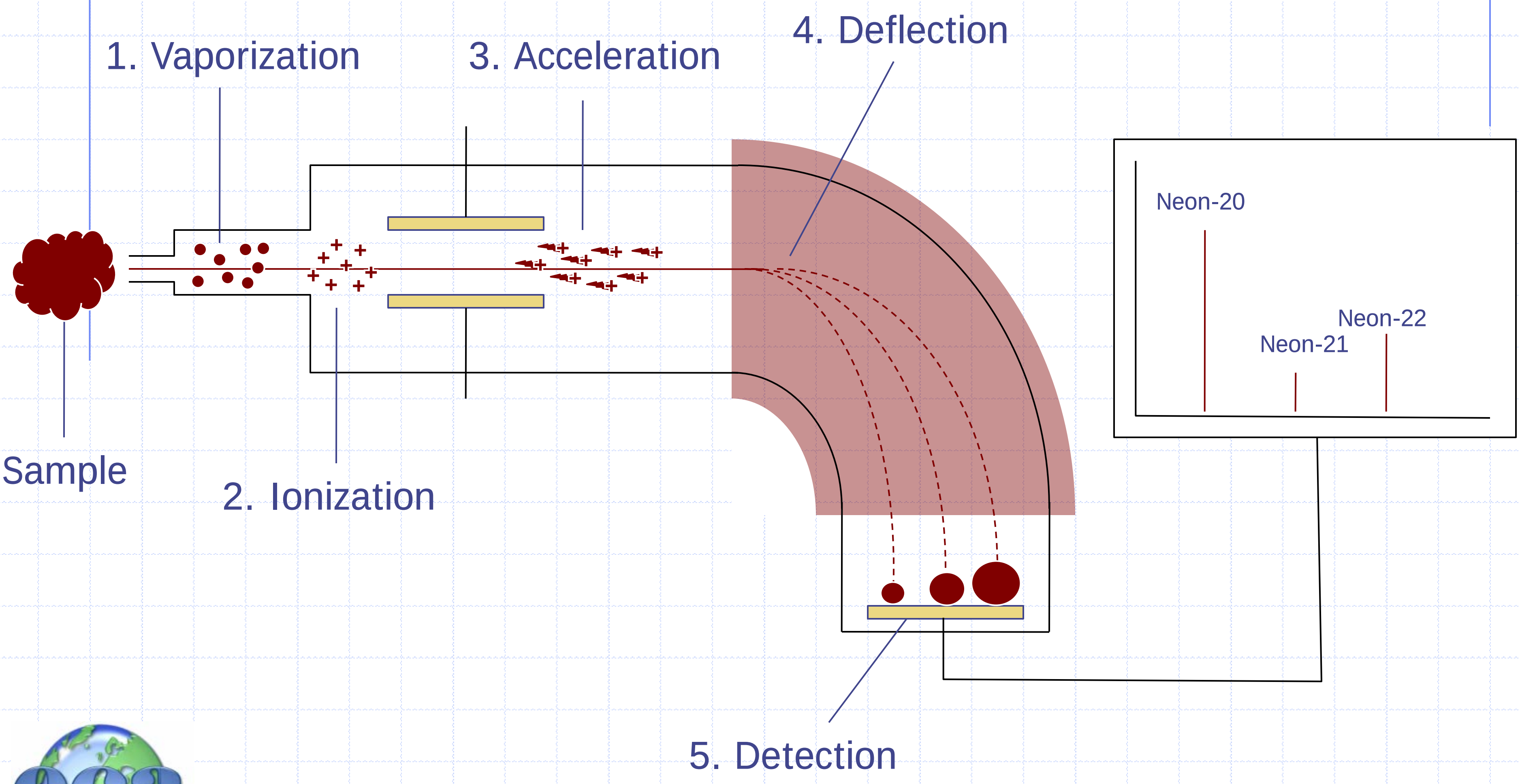
2.2.1 – Operation of Mass Spec

- 2.2.1 – Describe and explain the operation of a mass spectrometer
- What's it for? A **mass spectrometer** allows chemists to determine:
  - Relative atomic masses of atoms
  - Relative molecular masses of compounds
  - Structure of molecules
- How? By splitting up atoms, isotopes or molecules by their mass to charge ratio

2.2.1 – Diagram of a Mass Spec



2.2.1 – Steps of a Mass Spec



2.2.1 – Explanation of MS steps

- **1. Vaporization**: sample is energized to the state of a gas
- **2. Ionization:** gas is bombarded with high-speed electrons, making uni-positive (+1 charge) ions
  - $M(g) + e^- \rightarrow M^+(g) + 2e^-$
  - All ions in the MS will have the same charge, diff mass
- **3. Acceleration:** the electric field accelerates the positive ions
- **4: Deflection:** a strong magnetic field deflects the particles based on their mass-to-charge (m/z) ratio
- **5: Detection:** a detector counts the numbers of each of the different ions that impact upon it, providing a measure of the percentage abundance of each isotope

2.2.2 – What can we use MS data for?

- 2.2.2 – Describe how the mass spectrometer may be used to determine relative atomic mass using the ^{12}C (carbon-12) scale.
- Elements in the Periodic table have:
  - **Chemical Symbol**
  - **Atomic Number** (protons)
  - **Relative Atomic Mass** (A_r is NOT mass number)

10
Ne
20.18

- The majority of compounds exist as isotopes in a fixed proportion where each isotope has a different mass number. A weighted average of the abundance of each would give the A_r

2.2.2 – Relative Atomic Mass

- The weighted average (A_r) is only given a value compared to the mass of the carbon-12 atom
- 1/12th of carbon 12 would be one unit!
- So it's simply the weighted average divided by one!
- $A_r = \dfrac{weighted\ average\ mass\ of\ isotopes\ of\ the\ element}{\frac{1}{12} x\ the\ mass\ of\ one\ atom\ of\ carbon-12}$
- Use chlorine as an example:
  - Chlorine-35 = 75%
  - Chlorine-37 = 25%
  - Before we calculate, what number (35,37) should the weighted average be closer to?

2.2.2 – Simple A_r Calculation

- A_r Cl = (0.75 x 35amu) + (0.25 x 37amu)
- A_r Cl = 35.5 g/mol

- What is an **amu**?
  - Atomic Mass Units (1/12th of the carbon mass)
  - The units are grams per mole (**g/mol**)

- Now try the ones on your notes…..

2.2.3 – Non-integer A_r Calcs

- 2.2.3 – Calculate non-integer relative atomic masses and abundance of isotopes from given data
- The relative atomic mass (A_r) of Gallium is 69.7 g/mol. There are two stable isotopes ^{69}Ga and ^{71}Ga, calculate the percentage abundance of each:

2.2.3 – Find % Example

- The relative atomic mass (A_r) of Gallium is 69.7 g/mol. There are two stable isotopes ^{69}Ga and ^{71}Ga, calculate the percentage abundance of each:
- If $^{69}Ga\% = (x)$; then $^{71}Ga\% = (1-x)$
- $69.7 = (69x) + (71(1-x))$
- $69.7 = 69x + 71 – 71x$
- $-1.3 = -2x$
- $x = 0.65 = 65\%$ ^{69}Ga , 35% ^{71}Ga

- This is simple algebra, let's try some examples.....

1.2.4-5: Empirical/Molecular Formulas

- 1.2.4 – Distinguish between the terms empirical formula and molecular formula
- 1.2.5 – Determine the empirical formula from the percentage composition ~~or from other experimental data~~
- The **empirical formula** of a substance is the lowest whole number ratio of elements in the compound (simplified, like CH_2O)
- The **molecular formula** of a substance is the actual numbers of elements (like $C_6H_{12}O_6$)

1.2.5 – Using MS data to find the empirical formula

- Determine the empirical formula of a compound with 79.9% Carbon and 20.1% Hydrogen
- 1. Assume the % to be grams (out of 100g sample)
- 2. Convert grams of each element to moles using the molar mass (g/mol) (we will cover soon!)
- 3. Write the equation with mole ratios
- 4. Divide by the smallest # of moles
- 5. If needed, multiply until all have whole numbers

1.2.5: % to Empirical Example

- Determine the empirical formula of a compound with 79.9% Carbon and 20.1% Hydrogen
- 79.9% C = 79.9g C x $\frac{1 mol\ C}{12.01\ g\ C}$ = 6.65 mol C
- 20.1% H = 20.1g H x $\frac{1\ mol\ H}{1.01\ g\ H}$ = 19.9 mol H
- $C_{6.65}H_{19.9}$ / 6.65 = $CH_{2.99}$
- Round off 2.99 to 3, so we have **CH_3** as our **empirical formula**
- BUT, this is not the correct molecular formula....

1.2.5: Find Molecular from Empirical

- In order to find the molecular formula from the empirical formula you need more information to be given or found experimentally.
- So, if you were told that your molecular compound (that has an empirical formula of CH_3) has a molecular mass of 30.08, what would the molecular formula be?
- $CH_3 = (12.01 + (1.01x3)) = 15.04$ g/mol
- $30.08 = 15.04 \times 2$ so, $CH_3 \times 2 = C_2H_6$
  - **C_2H_6** is your **molecular formula**!

2.2.3: Find % Composition from Empirical or Molecular Formulas

- To backtrack, if you know the molecular formula to be C_2H_6, find the percentage composition of each compound. (This is theoretical, whereas Mass Spec data would be experimental)
- $\% = \dfrac{\#moles\ in\ formula\ x\ Molar\ Mass\ of\ element}{Molar\ Mass\ of\ Emperical\ (or\ Molecular)Formula} x100$
- $\%C = \dfrac{2\ x\ 12.01}{30.08}\ x\ 100 = 79.9\%\ C$
- $\%H = \dfrac{6\ x\ 1.01}{30.08}\ x\ 100 = 20.1\%\ H$